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Investigating the thermochemical conversion of biomass in a downdraft gasifier with a volatile break-up approach

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Abstract

An affordable, reliable and clean energy supply is the major challenge facing by the modern world. Biomass energy is playing a promising role to that, but gasification technology able to convert biomass efficiently to valuable gases for power and heat generation is a vital need. The aim of this study is to develop a robust computational fluid dynamics (CFD) model to better understand the gasification thermochemical processes of a selected biomass (rubber wood) in a 20 kW downdraft gasifier, which includes all the four zones, drying, pyrolysis, oxidation and reduction. A step-by-step approach is proposed to evaluate the composition of different species as a result of volatile break-up during gasification. Effect of the equivalence ratio on the synthesis gas composition is studied with results validated against a kinetic model. Further, in this study temperature profile in the gasifier at different equivalence ratio (ER) has been studied.

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Keywords: Biomass gasification; CFD; Downdraft gasifier; DPM model

1. Introduction

In today's world the demand of energy increasing day by day as the population is increasing and every country is looking for a new alternate source of energy. Biomass such as rubber wood, pine sawdust, rice husk, crops, forestry residues, corn, etc., are renewable energy resources which could be used for sustainable power and heat generation. Biomass gasification is a complex thermo-chemical process in which biomass is converted into synthesis gas mainly

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containing CO and H_2, with methane, ethylene and other pollutants. The synthesis gas can then be used as fuel in internal combustion engines, fuel cell and gas turbine. The lack of fundamental understanding of the design of downdraft gasifier for gasification of biomass is often based on empirical correlations and experiments in laboratory and pilot scale units. However, detailed models and numerical simulations will allow to address fundamental physical questions related to biomass conversion on a level not achievable with current capabilities of measurement techniques. At the end, validated and simulation models will help to design and optimize biomass conversion processes in downdraft gasifiers of industrial size.

There are numerous models available in the literature to simulate downdraft gasifier on different levels of accuracy and modeling depth. Generally, these can be categorized into two parts namely thermodynamic equilibrium and non-equilibrium or kinetic models. The equilibrium models also called zero dimensional models and widely used by various researchers [1-2]. But these models lack in clear understanding of gas-solid interface, temperature and concentration profile in the gasifier. On the other side, kinetic models [3-4] though account reaction kinetics and temperature of gasifier, still lack in comprehensively understanding of the biomass gasification process and the effects of the operating parameter and design parameter on the synthesis gas. Therefore, an advanced CFD based model may play a crucial role in the further development of this research and be useful for better understanding of the biomass gasification process and its design conditions. However, a very few CFD models available in the literature and most of the studies reported in the literature have been on the CFD simulation of entrained gasifier [1]. Two dimensional axisymmetric CFD model developed in a downdraft gasifier but in this model only oxidation zone was considered [2].

In this study more reactions are included compared to the previous study [3] and effect of temperature on the gasifier height at different ER are studied. Further, in this study effect of ER on the synthesis gas is studied which was not studied in the previous study [3].

One of the most important stages in numerical simulations of gasification is the distribution of species concentration during the devolatilization process occurring in a downdraft gasifier. Carbon, hydrogen and oxygen balance approach is available in literature [4], but in this study, for the first time, a volatile break-up approach is used to evaluate the species during the devoltilization. This approach conserves the mass of each of the elements as well as overall heat content in the solid fuel during this process.

2. Gasifier design and geometry

A schematic diagram of a downdraft gasifier is shown in Fig 1. The gasifier design parameters are taken from a recent study that focused on the development of an integrated kinetic model [5]. This kinetic model was tested with experimental results, and proposed the optimum design parameter for a downdraft gasifier used in this study. Air is injected from the combustion zone while rubber wood is feed from the top of the gasifier.

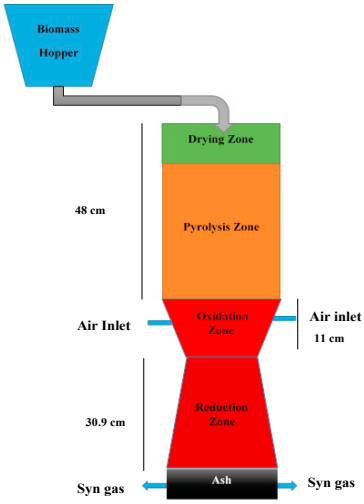

Fig. 1: Schematic of the downdraft gasifier.

3. Model description

In the present work, a steady-state, two-dimensional, incompressible and turbulent flow with biomass reaction is studied numerically. Therefore, the steady-state time averaged Navier-Stokes, energy and species transport equations are solved. The main governing equations are summarised in Table 1.

Table 1. The basic conservation governing equations for DPM model [6]

Force balance:- $$\frac{\partial \overrightarrow{u_p}}{\partial t} = F_D\left(\vec{u} - \vec{u}_p\right) + \frac{\vec{g}\left(\rho_p - \rho\right)}{\rho_p} \quad (1)$$

Where, $F_D\left(\vec{u} - \overrightarrow{u_p}\right)$ is the drag force per unit particle mass and

$$F_D = \frac{18\mu C_D \,\mathrm{Re}}{24\rho_p {d_p}^2} \quad (2)$$

Here, $\vec{u}$ is the fluid phase velocity, $\overrightarrow{u_p}$ is the particle velocity, μ is the molecular viscosity of the fluid, ρ is the fluid density, ρ_p is the density of the particle and d_p is the particle diameter. Re is the relative Reynolds number, which is defined as:

$$\mathrm{Re} = \frac{\rho d_p \left|\overrightarrow{u_p} - \vec{u}\right|}{\mu} \quad (3)$$

Inert heating and cooling:- $$m_p c_p \frac{dT_p}{dt} = hA_p\left(T - T_p\right) + \varepsilon_p A_p \sigma\left({T_R}^4 - {T_p}^4\right) \quad (4)$$

Where m_p of the particle (kg), c_p is the heat capacity of the particle (J/kg-K), A_p is the surface area of the particle (m^2), T is the local temperature of the continuous phase (K), h is the convective heat transfer coefficient (W/m^2-K), ε_p is the particle emissivity, σ is the T_R is the radiation temperature.

Two competing rates (Kobayashi) model: -

$$\frac{m_v(t)}{\left(1 - f_{w,0}\right)m_{p,0} - m_a} = \int_0^t \left(\alpha_1 R_1 - \alpha_2 R_2\right) \exp\left(-\int_0^t \left(R_1 - R_2\right)dt\right)dt \quad (5)$$

$$R_1 = a_1 e^{-\left(\frac{E_1}{RT_p}\right)}, R_2 = A_2 e^{-\left(\frac{E2}{RT_p}\right)}$$

$m_v(t)$ is the volatile yield up to time t, $m_{p,0}$ is the initial particle mass at injection, α_1, α_2 are the yield factors, m_a is the ash content in the particle.

Heat transfer during the devolatilization process: -

$$m_p c_p \frac{dT_p}{dt} = hA_p\left(T - T_p\right) + \frac{dm_p}{dt} h_{fg} + \varepsilon_p A_p \sigma\left({T_R}^4 - {T_p}^4\right) \quad (6)$$

Heat transfer during the char combustion process: -

$$m_p c_p \frac{dT_p}{dt} = hA_p\left(T - T_p\right) + f_h \frac{dm_p}{dt} H_{reac} + \varepsilon_p A_p \sigma\left({T_R}^4 - {T_p}^4\right) \quad (7)$$

The flow of rubber wood particles is modelled by a Lagrangian approach called discrete phase model. In this model the trajectories of rubber wood particles are tracked when they move through the continuous phase of the fluid. The

interaction between the discrete phase and the continuous phase is also taken into account by treating the heat and mass losses of the particles as the source term in the governing equations.

3.1 Thermochemical reactions

Volatiles, char and ash compositions released from the rubber wood decomposition is expressed by the following equation.

Rubber wood →Volatile + char + tar + ash (8)

Volatile→$x_1CO + x_2H_2 + x_3CO_2 + x_4CH_4 + x_5H_2O$ (9)

Where x_i is the number of moles species

$$\sum_i x_i = 1 \quad (10)$$

Rubber wood particles entering the gasifier undergo heating and as a result of that, the heat flowing around the rubber wood particles triggers a number of physical and chemical reactions. In the downdraft gasifier there are four different zones namely drying, pyrolysis, combustion and reduction. The oxidation and reduction zone reactions are given in Table 2.

3.2 Volatile break-up method

Volatile break-up approach developed in this work assumes that the volatile from the rubber wood consisting of carbon (C), hydrogen (H), oxygen (O), nitrogen (N) and sulphur (S), which are initially converted to a pseudo gas phase species, referred to as volatile using a devolatilization model. A gas phase volatile break-up reaction (9) is added to convert this gaseous volatile to several other gas phase species. Stoichiometric coefficients x_1, x_2, x_3, x_4 and x_5 for the resultant species are calculated from the obtained mass fractions and molecular weights of these species [3]. Using the current approach, a subroutine script is written to automatically calculate the stoichiometric coefficients of the volatile break-up reaction and integrated with the gasification simulation performed on ANSYS FLUENT.

Table 2. Reactions used in the oxidation and reduction zones

Oxidation zone reactions

	Reactions	*A*	*E* (kJ/mol)	Temp(exponent)	Reference
R1	$2C+O_2 \rightarrow 2CO$	147000	112.99	1	[7]
R2	$CO+0.5O_2 \rightarrow CO_2$	1.0e+10	126	0	[8]
R3	$2H_2+0.5O_2 \rightarrow 2H_2O$	2.2e+09	109	0	[8]
R4	$CH_4+1.5O_2 \rightarrow CO+2H_2O$	4.4e+11	126	0	[8]

Reduction zone reactions

	Reactions	*A*	*E* (kJ/mol)	Temp(exponent)	Reference
R5	$C+CO_2 \rightarrow 2CO$	8.268	188.2	1	[7]
R6	$C+H_2O \rightarrow CO+H_2$	8.268	188.2	1	[7]
R7	$0.5C+H_2 \rightarrow 0.5CH_4$	8.8894e-06	67.16	1	[7]
R8	$CH_4+H_2O \rightarrow CO+3H_2$	3e+08	125	0	[8]
R9	$CO+H_2O \rightarrow CO_2+H_2$	2.35e+10	288	0	[9]
R10	$CO_2+H_2 \rightarrow CO+H_2O$	1.785e+12	326	0	[9]

3.3 Boundary conditions

The boundary conditions for the simulation set up of the computational model are the same as those used in the kinetic model [5]. Namely, the mass flow rate of rubber wood is 3.65 kg/hr. The initial temperature of rubber wood and air are 300 K and 600 K respectively. The ultimate and proximate analysis data of rubber wood are given in Table 3.

Table 3. Characterization of rubber wood [10]

Ultimate analysis (wt% dry basis)		Proximate analysis (wt % dry basis)	
C	50.6	Volatile matter	81.1
H	6.5	Fixed carbon	19.2
O	42	Ash	0.7
N	0.2	Moisture content (wt % wet basis)	18.5
S	0	Higher heating value (kJ/kg)	20540

4. Simulation setup

A pressure-velocity coupling algorithm was used to solve the governing equations in association with the boundary conditions (ANSYS FLUENT v15). In which, the spatial discretization pressure was solved by the PRESTO with a second order upwind scheme for the momentum equations. The first order upwind scheme was used to solve the convection and diffusion fluxes. Initially, a grid dependency on the simulated results has been performed considering a computational grid cells of 29,420, 58,727 and 118,204. A negligible difference is observed between the results obtained by 58,727 and 118,204, hence the grid of 58,727 is chosen for all the simulation cases presented in the following section.

5. Results and discussion

Fig. 2 presents the simulation results for the temperature along the downdraft gasifier at different equivalent ratio (ER) varying from 0.35 to 0.6. As the ER value increases the temperature of oxidation increases due to increase of the concentration of O_2 in the oxidation zone, triggered by the char combustion reaction rate (R1) and volatile combustion reaction rates (R2-R4). The predicted temperature was in reasonable agreement with previous published results.

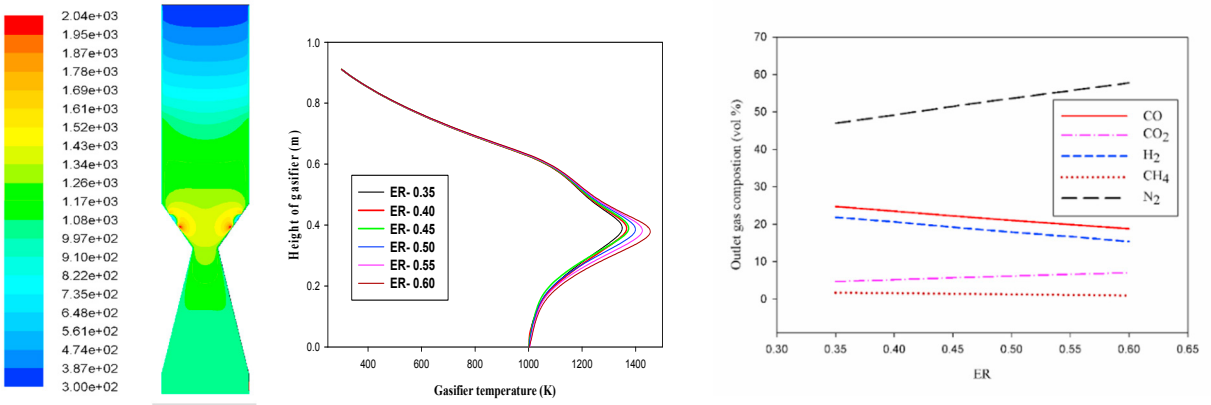

Fig. 2. Gasifier temperature and outlet gas composition at different equivalence ratios

A significant temperature drop is observed underneath the top of the gasifier because of the heat exchange between the cold feedstock and hot gasifying agent and also because of the endothermic drying and pyrolysis reactions. The temperature is then increased and becomes highest due to the exothermic combustion reactions occurring in the combustion zone. In the reduction zone however, mainly the endothermic reactions occur, and due to this the temperature in the reduction zone drop.

In the biomass gasification, ER is the most important parameter for gasifier design and it indicates the performance of the gasifier. The quality of gas obtained from the gasifier depends on the ER value, as seen in Fig.2. However, a relatively low value of equivalence ratio (e.g. ER<0.2) may result in many problems, including low heating value, excessive char formation and also incomplete gasification. On the other hand, a too high of ER will result in an excessive formation of products through complete combustion. A close examination in Figure 2 shows that the mole fraction of CO and H_2 decreases while CO_2 increases with the equivalence ratio. The CH_4 content also decreases with

the ER increase. Figure 3 depicts the comparison of the simulated outlet composition of gases (CO, CO_2, H_2, CH_4, and N_2) with those obtained by the kinetic model [5]. These plots reveal that simulated value of the outlet gas composition compares extremely well with the kinetic model prediction; hence the new modelling approach with volatile break up is proved to be reliable.

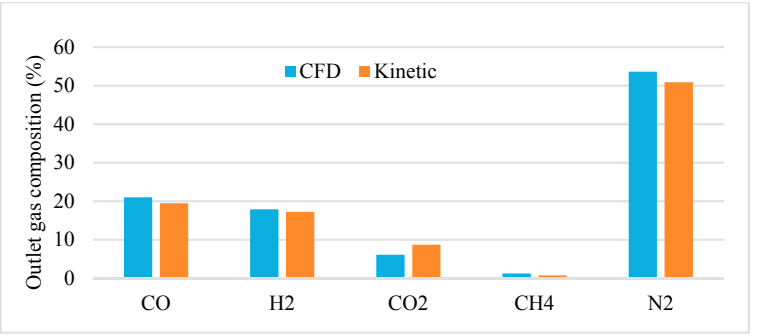

Fig.3. Comparison between the CFD and kinetic model predicted results

6. Conclusions

A two dimensional (2D) numerical model has been developed to simulate the rubber wood gasification process in a downdraft gasifier using Eulerian-Lagrange computational fluid dynamics (CFD) model. The simulated results reveal that the outlet gas composition of different species was closer to the kinetic model's results. Further, the model has been used to investigate the effect of equivalence ratio on the outlet gas composition. The present model is thus showing a promising way to simulate the biomass gasification in the downdraft gasifier.

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